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Autore	Albright Thomas A
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Molecular Orbitals of Diatomic Molecules and Electronegativity Perturbation; 6.1 Introduction; 6.2 Orbital Hybridization; 6.3 Molecular Orbitals of Diatomic Molecules; 6.4 Electronegativity Perturbation; 6.5 Photoelectron Spectroscopy and Through-Bond Conjugation; Problems; References
Chapter 7: Molecular Orbitals and Geometrical Perturbation7.1 Molecular Orbitals of AH2; 7.2 Geometrical Perturbation; 7.3 Walsh Diagrams; 7.4 Jahn-Teller Distortions; 7.4.1 First-Order Jahn-Teller Distortion; 7.4.2 Second-Order Jahn-Teller Distortion; 7.4.3 Three-Center Bonding; 7.5 Bond Orbitals and Photoelectron Spectra Of AH2 Molecules; Problems; References; Chapter 8: State Wavefunctions and State Energies; 8.1 Introduction; 8.2 The Molecular Hamiltonian and State Wavefunctions; 8.3 Fock Operator; 8.4 State Energy; 8.5 Excitation Energy; 8.6 Ionization Potential and Electron Affinity
8.7 Electron Density Distribution and Magnitudes of Coulomb and Exchange Repulsions8.8 Low versus High Spin States; 8.9 Electron-Electron Repulsion and Charged Species; 8.10 Configuration Interaction; 8.11 Toward More Quantitative Treatments; 8.12 The Density Functional Method; Problems; References; Chapter 9: Molecular Orbitals of Small Building Blocks; 9.1 Introduction; 9.2 The AH System; 9.3 Shapes of AH3 Systems; 9.4 -Bonding Effects of Ligands; 9.5 The AH4 System; 9.6 The AHn Series-Some Generalizations; Problems; References; Chapter 10: Molecules with Two Heavy Atoms; 10.1 Introduction
10.2 A2H6 Systems

Sommario/riassunto

Explains the underlying structure that unites all disciplines in chemistry Now in its second edition, this book explores organic, organometallic, inorganic, solid state, and materials chemistry, demonstrating how common molecular orbital situations arise throughout the whole chemical spectrum. The authors explore the relationships that enable readers to grasp the theory that underlies and connects traditional fields of study within chemistry, thereby providing a conceptual framework with which to think about chemical structure and reactivity problems. Orbital Interactions